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An efficient numerical solution strategy

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pH variation and influence in an autotrophic nitrogen removing biofilm system:

An efficient numerical solution strategy

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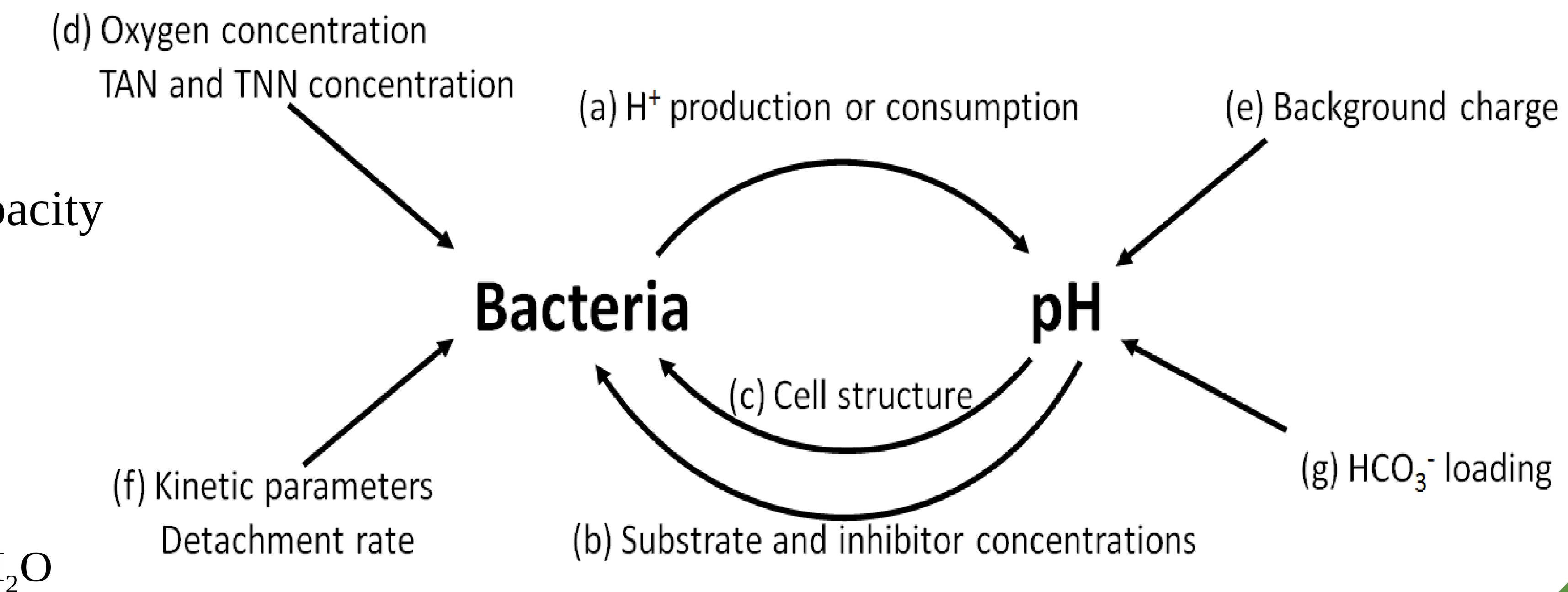
1. Introduction

pH impacts the nitritation and anammox processes and vice versa through: (a) H^+ production/consumption, (b) substrate and inhibitor speciation, (c) cell structure dependency, (d) substrate and inhibitor concentrations, (e) system background charge and distribution, (f) microbial activity, and (g) buffering capacity



Stoichiometry of microbial processes

Nitritation:

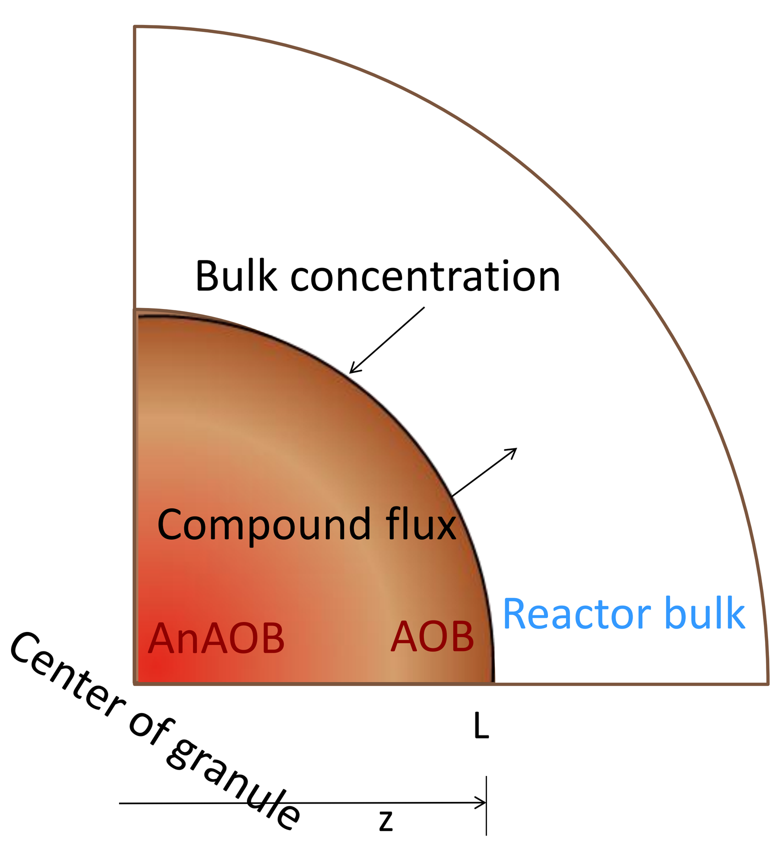
$$NH_4^+ + 1.38O_2 + 0.09CO_2 \rightarrow 0.018C_5H_7NO_2 + 0.98NO_2^- + 0.95H_2O + \underline{1.98H^+}$$

Anammox:

$$NH_4^+ + 1.32NO_2^- + 0.066HCO_3^- + \underline{0.13H^+} \rightarrow 1.02N_2 + 0.26NO_3^- + 0.066CH_2O_{0.5}N_{0.15} + 2.03H_2O$$

2. Methods and solution strategy

Model description



Biofilm mass balance

$$\frac{\partial(C_i V)}{\partial t} = \frac{\partial(j_i A)}{\partial z}dz + r_i dV$$

Reactor mass balance

$$\frac{dC_{i,bulk}}{dt} = \frac{Q_{in}C_{i,in} - Q_{out}C_{i,bulk}}{V_{reac}} - j_{Ci}\frac{A}{V_{reac}} + r_{i,bulk}$$

i = soluble or particulate compound
j = substrate flux
z = radial distance from the center of the granule
r_i = microbial growth and conversion
Q = flow
V_{reac} = reactor volume
A = biofilm surface area

New and fast numerical solution for pH calculation

A system of nine nonlinear equations was solved by a multi-dimensional Newton-Raphson method adapted from Luff et al. (2001) coupled with the granular biofilm model (left).

$$0 = TAN - (NH_4^+ + NH_3)$$
$$0 = TNN - (HNO_2 + NO_2^-)$$
$$0 = TIC - (CO_2 + HCO_3^- + CO_3^{2-})$$
$$0 = K_w - OH^- \cdot H^+$$
$$0 = K_{e,NH4} \cdot NH_4^+ - NH_3 \cdot H^+$$
$$0 = K_{e,HNO2} \cdot HNO_2 - NO_2^- \cdot H^+$$
$$0 = K_{e,CO2} \cdot CO_2 - HCO_3^- \cdot H^+$$
$$0 = K_{e,HCO3} \cdot HCO_3^- - CO_3^{2-} \cdot H^+$$
$$0 = Z^+ - NO_3^- - HCO_3^- - 2 \cdot CO_3^{2-} - NO_2^- - OH^- + NH_4^+ + H^+$$

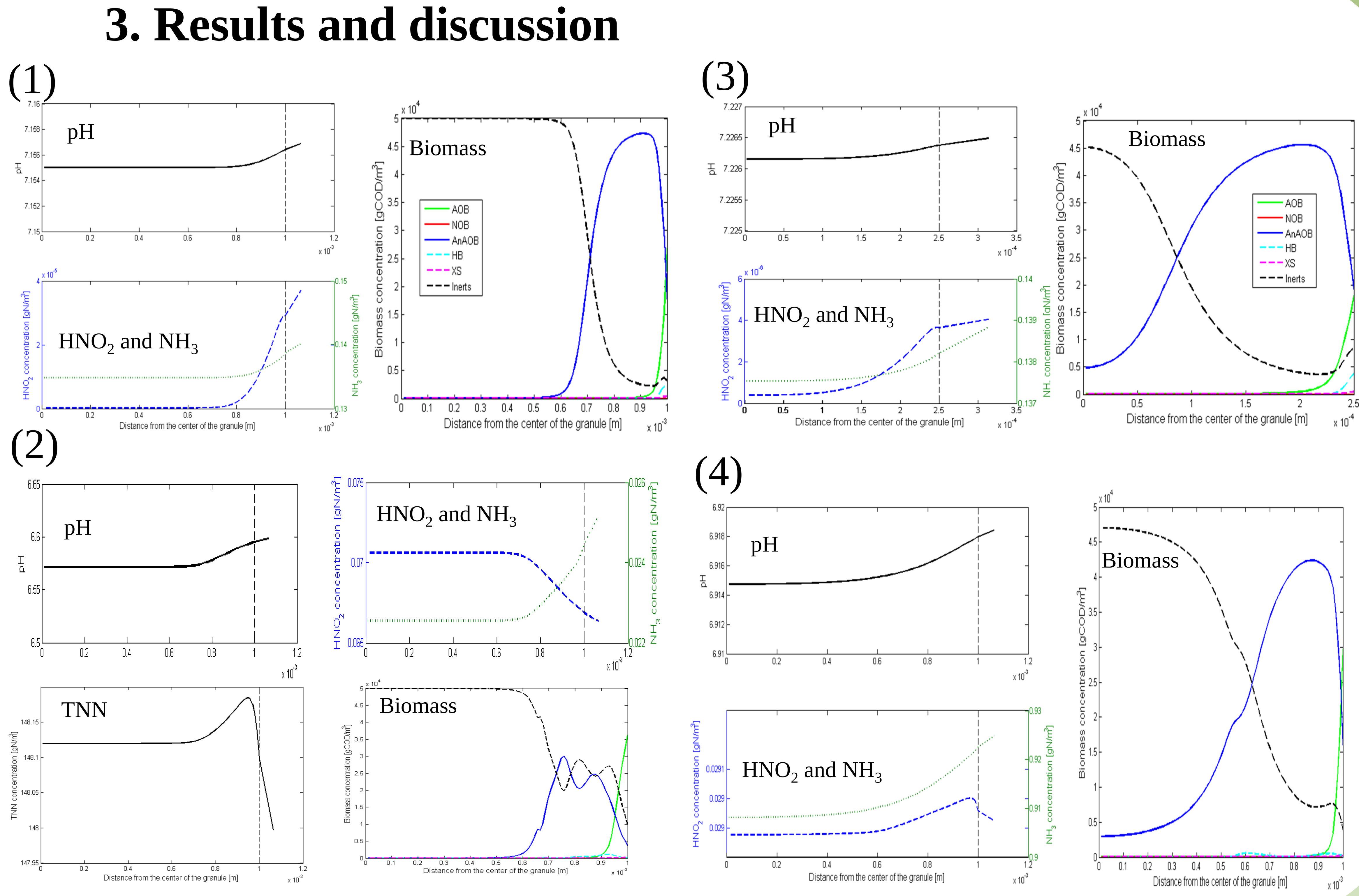
Because the above system was computationally heavy to solve and prone to errors, the pH was determined offline for the complete expected range of TAN, TNN, TIC and NO_3^-, prior to simulation. A lookup table was therefore constructed using multi-dimensional interpolation tools in the Matlab software.

Four scenarios representing different operating points were defined and simulated:
(1) Default (2) High oxygen loading (3) Smaller granules (4) High strength wastewater → N and oxygen loadings

3. Results and discussion

Findings

- pH solver was successfully constructed and implemented in the MATLAB software.
- Approximations of cell structure dependency on pH and the value of the background charge were needed to solve the model.
- The predicted pH profile showed decreasing pH with increasing depth into the biofilm in all scenarios, due to AOB presence in the outer layers.
- The background charge was found to have a great impact on the value and shape of the pH profile.
- More info on background charge effect and cell structure dependency, supported by experiments, is needed to make further progress.



References:
1. R. Luff et al. Comput. Geosci. **27**(2), 157-169 (2001).

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